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(54) **MASS SPECTROMETER UTILIZING MASS SPECTRAL DATABASE SEARCH FOR COMPOUND IDENTIFICATION**

(57) Real-time search (RTS) for mass spectrometry is described. In one instance, precursor ions generated from a sample are introduced into a mass spectrometer during an introduction period. The precursor ions are fragmented to form product ions, and a mass spectrum is acquired. During the introduction period, scores indicating the similarity between the mass spectrum and a candidate mass spectrum are identified. Based on the distribution of the scores, an action is performed.

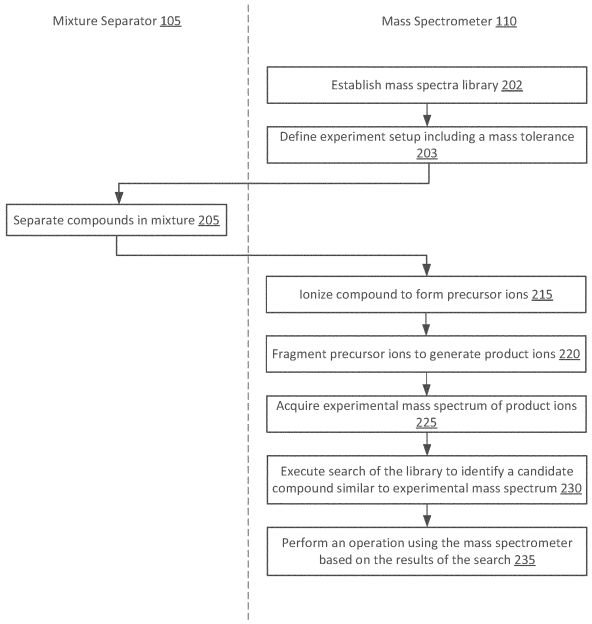


Figure 2

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EUROPEAN SEARCH REPORT

Application Number
EP 22 17 5613

DOCUMENTS CONSIDERED TO BE RELEVANT

Category	Citation of document with indication, where appropriate, of relevant passages	Relevant to claim	CLASSIFICATION OF THE APPLICATION (IPC)
X	US 2006/243900 A1 (OVERNEY GREGOR T [US] ET AL) 2 November 2006 (2006-11-02) * paragraph [0007] * * paragraph [0022] - paragraph [0029] * * paragraph [0031] - paragraph [0042] * * figures 1, 2A, 2B *	1,2,4-8, 10-16, 18-20	INV. H01J49/00 G01N33/50 G16B20/00
X	US 2011/288779 A1 (SATULOVSKY JAVIER E [US]) 24 November 2011 (2011-11-24) * paragraph [0030] - paragraph [0037] * * paragraph [0040] - paragraph [0086] * * figures 2, 3 *	1,2,4-8, 10-16, 18-20	
A	THOMAS DE VIJLDER ET AL: "A tutorial in small molecule identification via electrospray ionization-mass spectrometry: The practical art of structural elucidation", MASS SPECTROMETRY REVIEWS., vol. 37, no. 5, 9 November 2017 (2017-11-09), pages 607-629, XP055571302, US ISSN: 0277-7037, DOI: 10.1002/mas.21551 * paragraph [5.3.1] *	1,4,6,7, 13,14	TECHNICAL FIELDS SEARCHED (IPC) H01J G01N G06F G16B
A	US 8 445 843 B2 (KENNY DANIEL JAMES [GB]; MICROMASS LTD [GB]) 21 May 2013 (2013-05-21) * column 2, line 7 - line 22 *	2,8,18	
A	US 2005/098719 A1 (THOMSON BRUCE [CA]) 12 May 2005 (2005-05-12) * paragraph [0072] *	2,8,18	

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~~The present search report has been drawn up for all claims~~

Place of search	Date of completion of the search	Examiner
The Hague	7 October 2022	Cornelussen, Ronald

CATEGORY OF CITED DOCUMENTS

X : particularly relevant if taken alone
Y : particularly relevant if combined with another document of the same category
A : technological background
O : non-written disclosure
P : intermediate document

T : theory or principle underlying the invention
E : earlier patent document, but published on, or after the filing date
D : document cited in the application
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EP 22 17 5613

DOCUMENTS CONSIDERED TO BE RELEVANT

Category	Citation of document with indication, where appropriate, of relevant passages	Relevant to claim	CLASSIFICATION OF THE APPLICATION (IPC)
A	US 2003/162221 A1 (BADER GARY [CA] ET AL) 28 August 2003 (2003-08-28) * paragraph [0121] *	2,8,18	
			TECHNICAL FIELDS SEARCHED (IPC)

~~The present search report has been drawn up for all claims~~

Place of search	Date of completion of the search	Examiner
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X : particularly relevant if taken alone
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CLAIMS INCURRING FEES

The present European patent application comprised at the time of filing claims for which payment was due.

☐ Only part of the claims have been paid within the prescribed time limit. The present European search report has been drawn up for those claims for which no payment was due and for those claims for which claims fees have been paid, namely claim(s):

☐ No claims fees have been paid within the prescribed time limit. The present European search report has been drawn up for those claims for which no payment was due.

LACK OF UNITY OF INVENTION

The Search Division considers that the present European patent application does not comply with the requirements of unity of invention and relates to several inventions or groups of inventions, namely:

see sheet B

☐ All further search fees have been paid within the fixed time limit. The present European search report has been drawn up for all claims.

☐ As all searchable claims could be searched without effort justifying an additional fee, the Search Division did not invite payment of any additional fee.

☐ Only part of the further search fees have been paid within the fixed time limit. The present European search report has been drawn up for those parts of the European patent application which relate to the inventions in respect of which search fees have been paid, namely claims:

☒ None of the further search fees have been paid within the fixed time limit. The present European search report has been drawn up for those parts of the European patent application which relate to the invention first mentioned in the claims, namely claims:

1, 2, 4-8, 11-16, 18, 20(completely); 10, 19(partially)

☐ The present supplementary European search report has been drawn up for those parts of the European patent application which relate to the invention first mentioned in the claims (Rule 164 (1) EPC).

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LACK OF UNITY OF INVENTION
SHEET B

Application Number
EP 22 17 5613

The Search Division considers that the present European patent application does not comply with the requirements of unity of invention and relates to several inventions or groups of inventions, namely:

1. claims: 1, 2, 4–8, 11–16, 18, 20(completely); 10, 19(partially)

   Mass spectrometer and method of operating a mass spectrometer. While the ions are generated, a score that indicates a similarity between measured spectra and spectra of candidate compounds are determined. Based on this score, an action is performed on the precursor ions or the product ions. The action includes performing MS3 on the product ions.

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2. claims: 3, 9, 17(completely); 10, 19(partially)

   The action includes adjusting operational parameters of a fragmentation cell and fragmenting the precursor ions or the product ions with the fragmentation cell using the operational parameters.

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3. claims: 10, 19(all partially)

   The action includes performing an alternative dissociation technique on the same precursor ions or the product ions.

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4. claims: 10, 19(all partially)

   The action includes performing a reverse polarity MS scan.

ANNEX TO THE EUROPEAN SEARCH REPORT ON EUROPEAN PATENT APPLICATION NO. EP 22 17 5613

This annex lists the patent family members relating to the patent documents cited in the above-mentioned European search report. The members are as contained in the European Patent Office EDP file on
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07-10-2022

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For more details about this annex : see Official Journal of the European Patent Office, No. 12/82